

We claim:

1. A monocyclopentadienyl complex comprising the structural feature of the formula  $\text{Cp-Y}_m\text{M}^{\text{A}}$  (I), where the variables have the following meanings:

Cp is a cyclopentadienyl system having an aryl substituent,

Y is a substituent which is bound to Cp and contains at least one uncharged donor containing at least one atom of group 15 or 16 of the Periodic Table,

$\text{M}^{\text{A}}$  is titanium, zirconium, hafnium, vanadium, niobium, tantalum, chromium, molybdenum or tungsten or an element of group 3 of the Periodic Table and the lanthanides and

m is 1, 2 or 3.

2. A monocyclopentadienyl complex as claimed in claim 1 having the formula  $\text{Cp-Y}_m\text{M}^{\text{A}}\text{X}_n^{\text{A}}$  (V), where the variables have the following meanings:

Cp is a cyclopentadienyl system having an aryl substituent,

Y is a substituent which is bound to Cp and contains at least one uncharged donor containing at least one atom of group 15 or 16 of the Periodic Table,

$\text{M}^{\text{A}}$  is titanium, zirconium, hafnium, vanadium, niobium, tantalum, chromium, molybdenum or tungsten or an element of group 3 of the Periodic Table and the lanthanides and

m is 1, 2 or 3,

$\text{X}^{\text{A}}$  the radicals  $\text{X}^{\text{A}}$  are each, independently of one another, fluorine, chlorine, bromine, iodine, hydrogen,  $\text{C}_1\text{-C}_{10}\text{-alkyl}$ ,  $\text{C}_2\text{-C}_{10}\text{-alkenyl}$ ,  $\text{C}_6\text{-C}_{20}\text{-aryl}$ , alkylaryl having 1-10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part,  $\text{NR}^{23\text{A}}\text{R}^{24\text{A}}$ ,  $\text{OR}^{23\text{A}}$ ,  $\text{SR}^{23\text{A}}$ ,  $\text{SO}_3\text{R}^{23\text{A}}$ ,  $\text{OC(O)R}^{23\text{A}}$ , CN, SCN,  $\beta$ -diketonate, CO,  $\text{BF}_4^-$ ,  $\text{PF}_6^-$  or bulky noncoordinating anions or two radicals  $\text{X}^{\text{A}}$  form a substituted or unsubstituted diene ligand, in particular a 1,3-diene ligand, and the radicals  $\text{X}^{\text{A}}$  may be joined to one another,

$\text{R}^{23\text{A}}\text{-R}^{24\text{A}}$  are each, independently of one another, hydrogen,  $\text{C}_1\text{-C}_{20}\text{-alkyl}$ ,  $\text{C}_2\text{-C}_{20}\text{-alkenyl}$ ,  $\text{C}_6\text{-C}_{20}\text{-aryl}$ , alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part,  $\text{SiR}^{25\text{A}}_3$ , where the organic radicals  $\text{R}^{23\text{A}}\text{-R}^{24\text{A}}$  may also

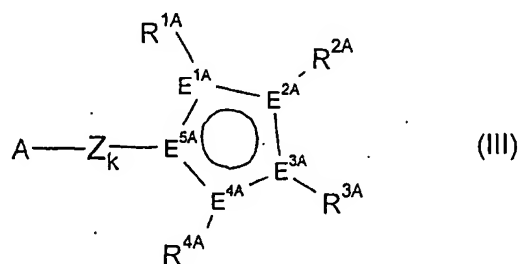
be substituted by halogens or nitrogen- and oxygen-containing groups and two radicals  $R^{23A}$ - $R^{24A}$  may also be joined to form a five- or six-membered ring,

$R^{25A}$  the radicals  $R^{25A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two radicals  $R^{25A}$  may also be joined to form a five- or six-membered ring and

n is 1, 2, or 3.

3. A monocyclopentadienyl complex as claimed in claim 1 or 2 in which Y is formed by the group  $-Z_k-A-$  and together with the cyclopentadienyl system Cp and  $M^A$  forms a monocyclopentadienyl complex comprising the structural element of the formula  $Cp-Z_k-A-M^A$  (II), where the variables have the following meanings:

$Cp-Z_k-A$



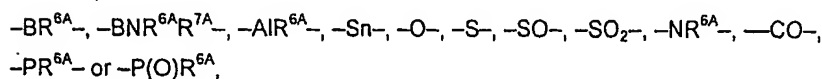
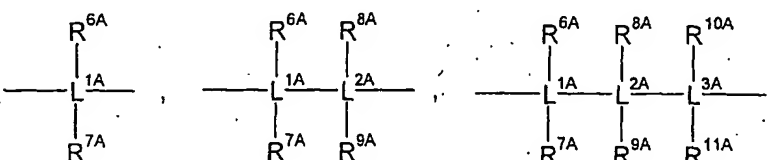
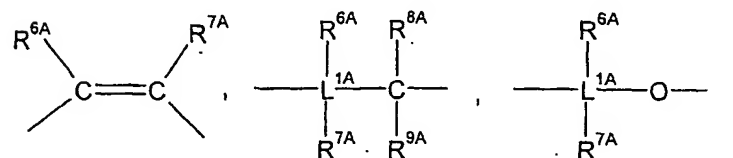
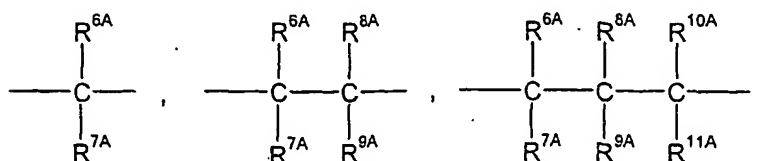
Where the variables have the following meanings:

$E^{1A}$ - $E^{5A}$  are each carbon or not more than one  $E^{1A}$  to  $E^{5A}$  is phosphorus,

$R^{1A}$ - $R^{4A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{22}$ -alkyl,  $C_2$ - $C_{22}$ -alkenyl,  $C_6$ - $C_{22}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl radical and 6-20 carbon atoms in the aryl radical,  $NR^{5A}_2$ ,  $N(SiR^{5A}_3)_2$ ,  $OR^{5A}$ ,  $OSiR^{5A}_3$ ,  $SiR^{5A}_3$ ,  $BR^{5A}_2$ , where the organic radicals  $R^{1A}$ - $R^{4A}$  may also be substituted by halogens and two vicinal radicals  $R^{1A}$ - $R^{4A}$  may also be joined to form a five-, six- or seven-membered ring, and/or two vicinal radicals  $R^{1A}$ - $R^{4A}$  are joined to form a five-, six- or seven-membered heterocycle which contains at least one atom from the group consisting of N, P, O or S and at least one  $R^{1A}$ - $R^{4A}$  is a  $C_6$ - $C_{22}$ -aryl, where the aryl may also be substituted by N-, P-, O- or S-containing substituents,  $C_1$ - $C_{22}$ -alkyl,  $C_2$ - $C_{22}$ -alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms,

$R^{5A}$  the radicals  $R^{5A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals  $R^{5A}$  may also be joined to form a five- or six-membered ring,

Z is a divalent bridge between A and Cp selected from the group consisting of



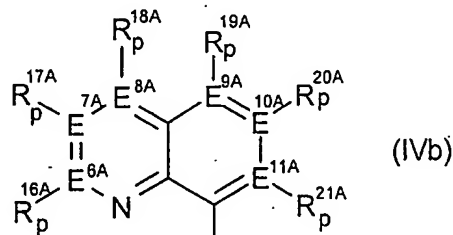
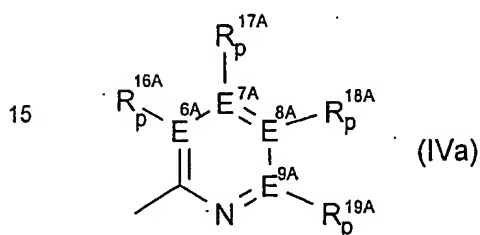
where

$L^{1A}$ - $L^{3A}$  are each, independently of one another, silicon or germanium,

$R^{6A}$ - $R^{11A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or  $SiR^{12A}_3$ , where the organic radicals  $R^{6A}$ - $R^{11A}$  may also be substituted by halogens and two geminal or vicinal radicals  $R^{6A}$ - $R^{11A}$  may also be joined to form a five- or six-membered ring and

$R^{12A}$  the radicals  $R^{12A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl or alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part,  $C_1$ - $C_{10}$ -alkoxy or  $C_6$ - $C_{10}$ -aryloxy and two radicals  $R^{12A}$  may also be joined to form a five- or six-membered ring, and

- A is an uncharged donor group containing one or more atoms of group 15 and/or 16 of the Periodic Table of the Elements or a carbene, preferably an unsubstituted, substituted or fused, heteroaromatic ring system,
- 5  $M^A$  is a metal selected from the group consisting of titanium in the oxidation state 3, vanadium, chromium, molybdenum and tungsten and
- k is 0 or 1.
- 10 4. A monocyclopentadienyl complex as claimed in any of claims 1 to 3 in which A is a group of the formula (IVa) or (IVb):



20 , where  
 $E^{6A}-E^{11A}$  are each, independently of one another, carbon or nitrogen,

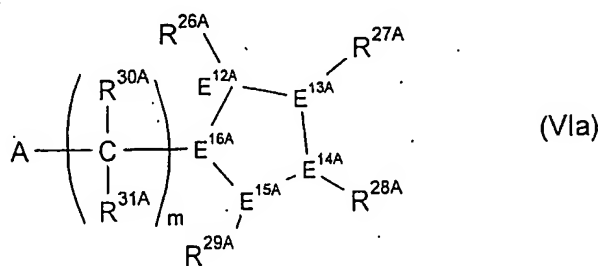
25  $R^{16A}-R^{21A}$  are each, independently of one another, hydrogen,  $C_1-C_{20}$ -alkyl,  $C_2-C_{20}$ -alkenyl,  $C_6-C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or  $SiR^{22A}_3$ , where the organic radicals  $R^{16A}-R^{21A}$  may also be substituted by halogens or nitrogen and further  $C_1-C_{20}$ -alkyl,  $C_2-C_{20}$ -alkenyl,  $C_6-C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or  $SiR^{22A}_3$  groups and two vicinal radicals  $R^{16A}-R^{21A}$  or  $R^{16A}$  and Z may also be joined to form a five- or six-membered ring and

30  $R^{22A}$  the radicals  $R^{22A}$  are each, independently of one another, hydrogen,  $C_1-C_{20}$ -alkyl,  $C_2-C_{20}$ -alkenyl,  $C_6-C_{20}$ -aryl or alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two radicals  $R^{22A}$  may also be joined to form a five- or six-membered ring and

35 p is 0 when  $E^{6A}-E^{11A}$  is nitrogen and is 1 when  $E^{6A}-E^{11A}$  is carbon.

- 40 5. A monocyclopentadienyl complex as claimed in claim 3 or 4 in which -Z-A and the aryl substituent are in the 1,3-positions relative to one another.

6. A catalyst system for olefin polymerization comprising
- A) at least one monocyclopentadienyl complex according to claims 1 to 5,
  - B) optionally an organic or inorganic support,
  - C) optionally one or more activating compounds,
  - D) optionally further catalysts suitable for olefin polymerization and
  - E) optionally one or more metal compounds containing a metal of group 1, 2 or 13 of the Periodic Table.
7. A prepolymerized catalyst system comprising a catalyst system as claimed in claim 6 and one or more linear C<sub>2</sub>-C<sub>10</sub>-1-alkenes polymerized onto it in a mass ratio of from 1:0.1 to 1:1 000 based on the catalyst system.
8. The use of a catalyst system as claimed in claim 6 or 7 for the polymerization or copolymerization of olefins.
9. A process for preparing polyolefins by polymerization or copolymerization of olefins in the presence of a catalyst system as claimed in claim 6 or 7.
10. A process for preparing cyclopentadiene systems of the formula (VIa),



where the variables have the following meanings:

E<sup>12A</sup>-E<sup>16A</sup> are each carbon, with four adjacent E<sup>12A</sup>-E<sup>16A</sup> forming a conjugated diene system and the remaining E<sup>12A</sup>-E<sup>16A</sup> additionally bearing a hydrogen,

$R^{26A}$ - $R^{29A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part,  $NR^{32A}_2$ ,  $N(SiR^{32A}_3)_2$ ,  $OR^{32A}$ ,  $OSiR^{32A}_3$ ,  $BR^{32A}_2$ ,  $SiR^{32A}_3$ , where the organic radicals  $R^{26A}$ - $R^{29A}$  may also be substituted by halogens and two vicinal radicals  $R^{26A}$ - $R^{29A}$  may also be joined to form a five- or six-membered ring, and/or two vicinal radicals  $R^{26A}$ - $R^{29A}$  are joined to form a hetero-cycle which contains at least one atom from the group consisting of N, P, O or S,

$R^{30A}$ - $R^{31A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or  $SiR^{32A}_3$ , where the organic radicals  $R^{30A}$ - $R^{31A}$  may also be substituted by halogens and  $R^{30A}$  or  $R^{31A}$  and A may also be joined to form a five- or six-membered ring,

$R^{32A}$  the radicals  $R^{32A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals  $R^{32A}$  may also be joined to form a five- or six-membered ring,

m is 0, 1 or 2,

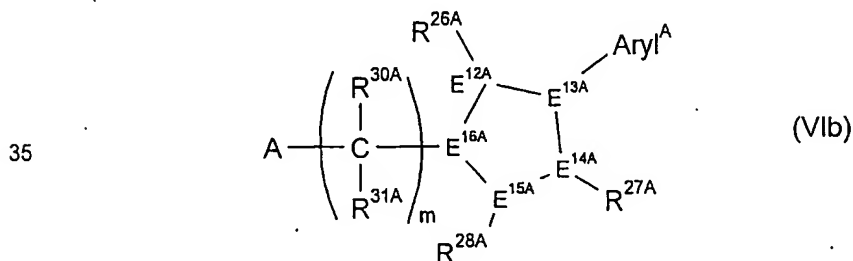
A is an uncharged donor group containing one or more atoms of group 15 and/or 16 of the Periodic Table of the Elements or a carbene, preferably an unsubstituted, substituted or fused, heteroaromatic ring system,

25

which comprises:

a) reacting an  $(A-(CR^{29A}R^{30A})_m)^-$  anion with a cyclopentanedione or a silyl ether of an enolised cyclopentanedione.

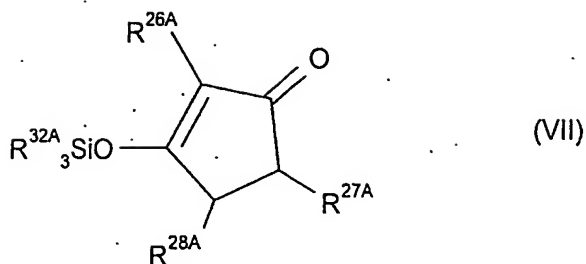
30 11. A process for preparing cyclopentadiene systems of the formula (VIb),



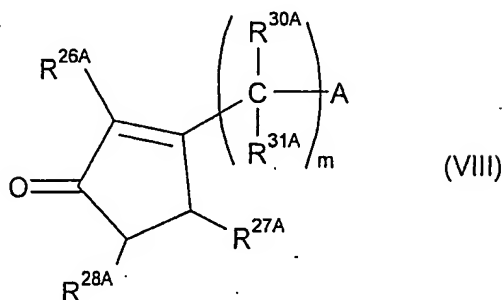
40 where the variables have the following meanings:

- $E^{12A}-E^{16A}$  are each carbon, with four adjacent  $E^{12A}-E^{16A}$  forming a conjugated diene system and the remaining  $E^{12A}-E^{16A}$  additionally bearing a hydrogen,
- $R^{26A}-R^{28A}$  are each, independently of one another, hydrogen,  $C_1-C_{20}$ -alkyl,  $C_2-C_{20}$ -alkenyl,  $C_6-C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part,  $SiR^{32A}_3$ , where the organic radicals  $R^{26A}-R^{28A}$  may also be substituted by halogens and two vicinal radicals  $R^{27A}-R^{28A}$  may also be joined to form a five- or six-membered ring, and/or two vicinal radicals  $R^{27A}-R^{28A}$  are joined to form a heterocycle which contains at least one atom from the group consisting of N, P, O or S,
- $R^{30A}-R^{31A}$  are each, independently of one another, hydrogen,  $C_1-C_{20}$ -alkyl,  $C_2-C_{20}$ -alkenyl,  $C_6-C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or  $SiR^{32A}_3$ , where the organic radicals  $R^{30A}-R^{31A}$  may also be substituted by halogens and  $R^{30A}$  or  $R^{31A}$  and A may also be joined to form a five- or six-membered ring,
- $R^{32A}$  the radicals  $R^{32A}$  are each, independently of one another, hydrogen,  $C_1-C_{20}$ -alkyl,  $C_2-C_{20}$ -alkenyl,  $C_6-C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals  $R^{32A}$  may also be joined to form a five- or six-membered ring,
- $Aryl^A$  is  $C_6-C_{22}$ -aryl, for example phenyl, naphthyl, biphenyl, anthracenyl or phenanthrenyl, which may also be substituted by N-, P-, O- or S-containing substituents,  $C_1-C_{22}$ -alkyl,  $C_2-C_{22}$ -alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms and
- m is 0 or 1,
- A is an unsubstituted, substituted or fused heteroaromatic ring system,
- which comprises:

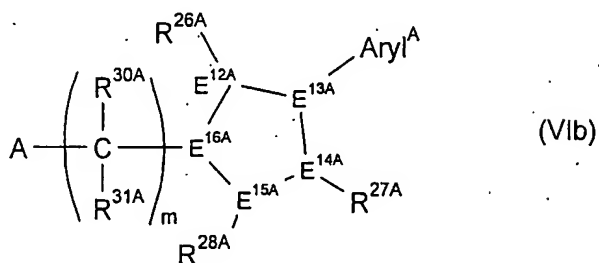
- a) reacting an  $(A-(CR^{30A}R^{31A})_m)^-$  anion with a cyclopentenone system of the formula (VII)



10 to form a cyclopentenone of the formula (VIII)



20 12. A cyclopentadiene system of the formula (Vib),



30 where the variables have the following meanings:

$E^{12A}-E^{16A}$  are each carbon, with four adjacent  $E^{12A}-E^{16A}$  forming a conjugated diene system and the remaining  $E^{12A}-E^{16A}$  additionally bearing a hydrogen,

35  $R^{26A}-R^{28A}$  are each, independently of one another, hydrogen,  $C_1-C_{20}$ -alkyl,  $C_2-C_{20}$ -alkenyl,  $C_6-C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part,  $SiR^{32A}_3$ , where the organic radicals  $R^{26A}-R^{28A}$  may also be substituted by halogens and two vicinal radicals  $R^{27A}-R^{28A}$  may also be joined to form a five- or six-membered ring, and/or two vicinal radicals  $R^{27A}-R^{28A}$  are joined to form a heterocycle which contains at least one atom from the group  
40 consisting of N, P, O or S,



5  $R^{30A}$ - $R^{31A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or  $SiR^{32A}_3$ , where the organic radicals  $R^{30A}$ - $R^{31A}$  may also be substituted by halogens and  $R^{30A}$  or  $R^{31A}$  and A may also be joined to form a five- or six-membered ring,

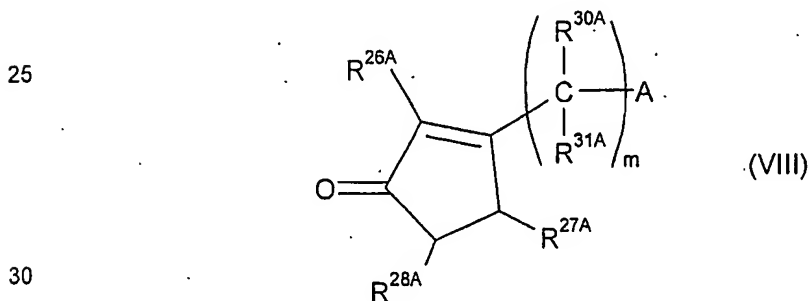
10  $R^{32A}$  the radicals  $R^{32A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals  $R^{32A}$  may also be joined to form a five- or six-membered ring,

15 Aryl<sup>A</sup> is  $C_6$ - $C_{22}$ -aryl, for example phenyl, naphthyl, biphenyl, anthracenyl or phenanthrenyl, which may also be substituted by N-, P-, O- or S-containing substituents,  $C_1$ - $C_{22}$ -alkyl,  $C_2$ - $C_{22}$ -alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms and

m is 0 or 1 and

20 A is an unsubstituted, substituted or fused heteroaromatic ring system.

13. A cyclopentenone of the formula (VIII)



where the variables have the following meanings:

35  $R^{26A}$ - $R^{28A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part,  $SiR^{32A}_3$ , where the organic radicals  $R^{26A}$ - $R^{28A}$  may also be substituted by halogens and two vicinal radicals  $R^{27A}$ - $R^{28A}$  may also be joined to form a five- or six-membered ring, and/or two vicinal radicals  $R^{27A}$ - $R^{28A}$  are joined to form a heterocycle which contains at least one atom from the group consisting of N, P, O or S,

40

5  $R^{30A}$ - $R^{31A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part or  $SiR^{32A}_3$ , where the organic radicals  $R^{30A}$ - $R^{31A}$  may also be substituted by halogens and  $R^{30A}$  or  $R^{31A}$  and A may also be joined to form a five- or six-membered ring,

10  $R^{32A}$  the radicals  $R^{32A}$  are each, independently of one another, hydrogen,  $C_1$ - $C_{20}$ -alkyl,  $C_2$ - $C_{20}$ -alkenyl,  $C_6$ - $C_{20}$ -aryl, alkylaryl having from 1 to 10 carbon atoms in the alkyl part and 6-20 carbon atoms in the aryl part and two geminal radicals  $R^{32A}$  may also be joined to form a five- or six-membered ring,

15 Aryl<sup>A</sup> is  $C_6$ - $C_{22}$ -aryl, for example phenyl, naphthyl, biphenyl, anthracenyl or phenanthrenyl, which may also be substituted by N-, P-, O- or S-containing substituents,  $C_1$ - $C_{22}$ -alkyl,  $C_2$ - $C_{22}$ -alkenyl, halogens or haloalkyls or haloaryls having 1-10 carbon atoms and

m is 0 or 1 and

20 A is an unsubstituted, substituted or fused heteroaromatic ring system.

25

30

35

40